KARNATAKA STATE WOMEN'S UNIVERSITY, VIJAYAPUR

Jnanashakti Campus, Torvi, Vijayapur

2017

2018-2019

A synoptic Note on

"Insilico drug designing studies of Phytochemicals Isolated from Launaea procumbens against diabetes mellitus"

Doctor of Philosophy

In

Bioinformatics

By

Miss. Indirabai .M .Beeraladinni

Under the Guidance of

Prof. S.B.Madagi

Professor

Department of Bioinformatics

KSAWU, Vijayapur

Contents:

1.0. Introduction

2.0. Aim and Objectives
3.0. Materials and methods
4.0. Expected outcome
5.0. References

Abstract:

Disease development is mainly caused by both environmental and genetic factors. Understanding how genetic factors influence the human diseases remains challenge. Diabetes is a chronic disease in which body unable to make enough insulin or to use insulin correctly. (Weir and Bonner-Weir,2004) Type 1 diabetes (T1D) is an autoimmune disease, where type 2 (T2D) and gestational diabetes (GDM) are considered metabolic disturbances. life style interventions, food habits, less physical activities, obesity and tensions are playing a vital role to understand the factors involved in the particular disease.

The present study focuses on plant extracts or phytochemicals role in diabetes management. This has been tried by many researchers, The phytochemicals involved in lowering blood sugar, developing eye sight and different mechanisms in reducing diabetes. By this study in the study plant few molecules may be used in diabetes management and they possess molecular mechanisms or involved in signal transduction to initiate the insulin production or utilization of blood glucose level bring down to normal stage(Govindappa, 2015).

The researchers have used different parts of the plant extracts or individual phytochemicals for antidiabetic activities. In this investigation we shall focus on assessing the antidiabetic activities of *Launaea procumbens* plant extracts role in reducing of diabetic problems.

Introduction:

When blood glucose level is too high it is called diabetes. High blood glucose can cause health problems over time**.** The number of diabetes population is rising day by day in world

wide. according to statistical data it was 108 million in 1980. The number of people with diabetes has risen 171 million in 2000. It increases 422 million in 2014 *(WHO).* It may double 366 million in 2030. In India it was 31.7 million in 2000, topped the world with the highest number of people with diabetes mellitus followed by China 20.8 million, with the United States 17.7 million in second and third place respectively. with a maximum increase in India. It is predicted that by 2030 diabetes mellitus may afflict up to 79.4 million individuals in India, while China 42.3 million and the United States 30.3 million. (Seema Abhijeet et al, 2014).

The main types of diabetes are type 1, type 2, and gestational. Diabetes mellitus is characterized by alterations in the metabolism of carbohydrate, fat and protein, is caused by a relative or absolute deficiency of insulin secretion and different levels of insulin resistance and it is resulting from both genetic predisposition and favoring environmental factors. In the patients, late complications develop consisting of alterations and failure of various organs (especially the non-insulin sensitive ones) including the eyes (retinopathy with vision loss), kidneys (nephropathy leading to renal failure), nerves (peripheral and autonomic neuropathy), heart and blood vessels (precocious and severe cardiovascular, cerebrovascular and peripheral vascular atherosclerosis(Govindappa, 2015) The Juices of different plant materials shown the increasing of eye sight, lowering blood glucose by 10-20%. (Durgacharan A. Bhagwat et.al, 2008)

Bioinformatics:

Bioinformatics is a multidisciplinary field it uses information technology, statistics, Mathematics, Physics and chemistry for storage, retrieval and analysis of biological data. on this aspect which can solves complicated biological problems in molecular and cellular level. For development of novel treatment strategies for diabetes, Phytochemical based study will helps to identify antidiabetic activity present in the plants. there are so many tools and techniques available in bioinformatics to check the ADMET and QSR properties.

Aim:

In-silico drug designing studies of phytochemicals isolated from Launaea procumbens against Diabetes Mellitus.

Objectives:

1. Extraction and isolation of phytochemicals from Launaea procumbens

2. Characterization and identification of isolated phytochemicals by spectral studies

3. Invitro antidiabetic activity of extracts and phytochemicals of study plants

4. Evaluation of anti-amylase activity of extracts and phytochemicals of study plants

5. In-silico drug designing studies of isolated phytochemicals

6. In-silico QSAR and ADME studies of potential compound.

Materials and method:

1.Medicinal plants from the vicinity of vijayapur district will be collected sequential shade dried

2. plant extract shall be subjected to column chromatography, pure compound isolated will be and then using different solvents will be subjected to Soxhlet extraction followed by rotatory flash evaporator and the extraction will be dried.

subjected for special studies by H.NMR, 13c-NMR, FT-IR and LC-MS. Based on spectral results compound structure will be elucidated.

3. Invitro glucose uptake assay will be carried out in yeast and in cell lines.

4. Invitro amylase inhibition assay will be carried out followed Beta-glucosidase inhibition assay will be carried out.

5.coputational drug designing studies of isolated compound will be carried out by molecular docking and simulation studies.

6.In-silico pharmacokinetics studies will be carried out by assessing QSAR and ADME properties of the isolated compound.

Expected outcome:

1. Diabetes is a metabolic disorder found in approximately 75% of the people It is commonly associated with obesity, insulin resistance (IR), and clinical hypoglycemia
2. hence need to find out inhibitors to inhibit the activity of the diabetes causing proteins.

3. A systematic *in silico* protocol of bioinformatics approaches is implemented and best docking complex is proposed as best inhibitor complex of the target.

4. And it may be good pharmacological properties and least docking score and ΔG score.

References:

1. Govindappa, J Diabetes Metab 2015 A Review on Role of Plant(s) Extracts and its Phytochemicals for the Management of Diabetes

2. *WHO*.

3. Seema Abhijeet Kaveeshwar1 et.al, 2014

4. Durgacharan A. Bhagwat et.al, 2008Anti-diabetic activity of leaf extract of Tridax procumbens.

5. Weir and Bonner-Weir (2004), Diabetes 53 Suppl 3: S16–21.

6. Varsha V Sonkamble et.al, 2015

7. Fazeela Mehaboob Begum SM et.al, 2017.